REPRESENTATIVE PATHWAY LENGTH FOR CONTAMINANT TRANSPORT IN PERFORMANCE ASSESSMENT MODELS

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Performance assessment models, in the context of high-level waste management, commonly incorporate a "representative" element concept as a simplification approach. For example, on the basis of a representative waste package, radionuclide release away from a single waste package is computed and scaled up to derive an estimate of the total release from an ensemble of waste packages. This computation is an approximation, as each waste package may release radionuclides at different rates controlled by local conditions in or around the waste package. This paper considers several approaches for defining an averaged property, length of transport pathway in this example, so that scaled-up releases are consistent with releases that would be computed by individually simulating each waste package. Results (total release rates) from a detailed formulation are compared to those considering common averages for the derivation of the representative property, and these can differ significantly. This implies that representative properties should be carefully selected in general. The example in this paper illustrates that, even in a simple case, detailed determination of an appropriate representative property can be a complex endeavor. This is particularly true for cases where the representative element (waste package in this example) is intended to summarize multiple properties that exhibit spatial variability. Therefore, depending on the intended use of the performance assessment model, elements may need to be included to explicitly model spatial variability.

I. BACKGROUND

Performance assessments are generally intended as tools to support decision making. In a performance assessment, a system is evaluated by comparing performance metrics calculated with a performance assessment model (e.g., total release rates, cumulative release rates, contaminant concentrations in groundwater, doses to a receptor) to corresponding safety thresholds. Performance assessments may become complex for systems subject to multiple safety thresholds. Performance assessment models may also become complex to account for factors that are important to compliance with safety standards, particularly if those factors exhibit variability and uncertainty. On the other hand, a low-complexity performance assessment model may be sufficient to satisfy the model intent if few factors control performance metrics and there is a single safety threshold.

Developing low-complexity performance assessment models is desirable for reasons such as reducing computational burden, maintaining consistency with limited available information, and achieving compatibility with intended model usage. Representative elements are commonly used to simplify the calculations. Representative elements are single components of a performance assessment model that are intended to summarize or consolidate multiple components of the real system. For example, a common approach for calculating radionuclide releases is to calculate releases from a single representative waste package, then scale up these releases to derive an estimate of the total release from an ensemble of waste packages. This computation is a simplification, as each waste package may release radionuclides at different rates controlled by local conditions in or around the waste package.

Using an example, this paper illustrates the challenges of defining an uncertain and variable property for use in a low-complexity performance assessment model. For the purposes of this example, the performance assessment model does not directly include property variability but represents it in an average sense. The performance assessment model considers property uncertainty by sampling the statistical properties representing property variability.

The example compares two approaches: (i) the representative-parameter approach (Method 1), in which an averaged property is directly estimated from the statistical representation of the physical parameter, and (ii) the equivalent-parameter approach (Method 2), in which the averaged property is indirectly estimated using equivalency requirements. The equivalency approach seeks to assure that releases directly calculated using an ensemble of individual waste packages with property variability considered are numerically equivalent to scaled-up releases calculated using the sampled equivalent parameter.

The length of a contaminant transport pathway between a waste package and a flowing fracture, which is tied to the separation between flowing fractures, is used for the example. The two approaches yield comparable results when transport in the pathway does not constrain release. When pathway transport does constrain release, the two methods calculate differing release rates with low transport-length variability and can yield results differing by more than an order of magnitude as transport-length variability increases.

The example highlights the need to carefully select and design representative elements to properly account for spatial variability. The example results suggest that it may be useful to consider multiple disaggregated elements in developing representative elements.

II. SYSTEM DESCRIPTION

The hypothetical radioactive waste disposal system considered in this analysis is consistent with the performance assessment model described in an accompanying paper.[1] The performance assessment model includes a source model, components computing radionuclide transport in geologic media, and a biosphere dose model. The source model includes descriptions of waste forms, radionuclide inventories, and waste form dissolution rates. The source model also incorporates abstractions for waste package failure, transport through a buffer material (a diffusive barrier that surrounds the waste packages), and transport through a drift and radionuclide discharge into nearby fractures. The radionuclide discharge is used as input to the geologic media transport computations. The analysis in this paper considers transport in the buffer material and transition region, the region in the drifts from the buffer material to the nearby fractures. The length of this transition region is the transport length of interest.

The waste packages of interest are distributed along the axis of a tunnel emplaced in sparsely fractured, low-permeability host rock (e.g., granite rock). The tunnel could be open or backfilled with crushed host rock or other natural or engineered material. The tunnel is assumed to be fully saturated with essentially stagnant groundwater (i.e., diffusion is the dominant transport process), but water in the fractures could move at faster rates. Each waste package is assumed to be located between two flowing fractures intercepting the tunnel (see Fig. 1). The flowing fractures are represented as planes perpendicular to the tunnel axis; not all fractures are necessarily flowing. Radionuclides diffusing away from the buffer material are transported toward the two closest flowing fractures (the region from the buffer material to a fracture is referred to as the transition region), in which radionuclides are held at low or zero concentration. As shown in Fig. 1, each waste package location is represented by two random variables, a fracture spacing (L) and a fraction of the distance between fractures (f).

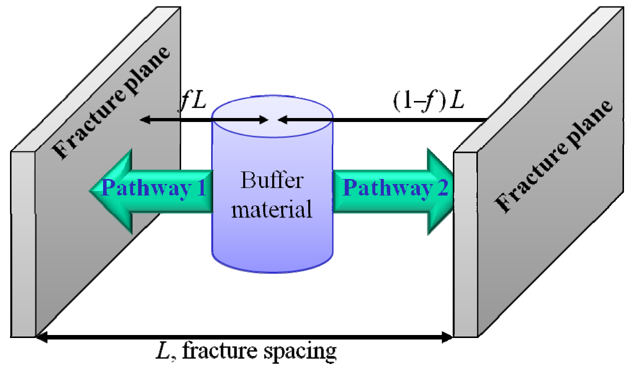

Fig 1. Representation of transport pathways. The fracture spacing, L, and the waste package placement fraction, f, are random variables.

Uncertainty and variability are inherent components in performance assessments, commonly evaluated through multiple Monte Carlo realizations.[2,3] Approaches for incorporating uncertainty and variability in performance assessments range from approaches that individually represent each waste package and transport pathway (rich in detail regarding extremes at the cost of very demanding computations and data needs) through methods that "integrate out" aspects of variability and uncertainty (reducing the computational burden and data requirements with a tradeoff of reduced detail regarding extremes). The entire range of approaches can, in principle, resolve the expected behavior of the ensemble of releases, with appropriate parameterization, because central tendency is a robust statistical measure.

Performance assessments commonly "integrate out" variability using representative parameters, often by directly averaging the parameter values. While straightforward, averaging can lead to biased estimates of performance metrics. We recommend developing the parameters for performance assessment using relevant performance metrics. For example, if the total release into the geosphere from the engineered barrier system is adopted as a performance metric, the representative length of the transport pathway should, when used to compute the radionuclide discharge into the fractures, yield a discharge that is equivalent to the expected value computed by explicitly considering all possible fracture separations and all possible waste package placements (i.e., integrating over L and f in Fig. 1). If such equivalence is possible, then total releases derived by scaling up the release from a representative waste package are accurately computed.

In the example problem, L is the physical variable exhibiting the largest range of spatial variability. We demonstrate the utility of the approach by comparing estimates using the common approach of using expected values of L and f over the range of spatial variability (i.e., Method 1, arithmetic and harmonic means) with the estimates directly considering variability (i.e., Method 2, equivalent parameter).

III. MODEL

The example uses a simple model for diffusive transport of radionuclides from a waste package to the natural system, consisting of two one-dimensional legs in series: one through the buffer material, and one in the transition region from the buffer to a flowing fracture via the emplacement opening and near-field host rock. The steady-state concentration profile is depicted in Fig. 2. Neglecting transient storage conservatively overestimates release to the natural system in the early stages after waste package failure. Assuming that the flowing fracture concentration is zero overestimates release rates, but only slightly when the fracture incoming concentration is much smaller than the concentration at the waste package.

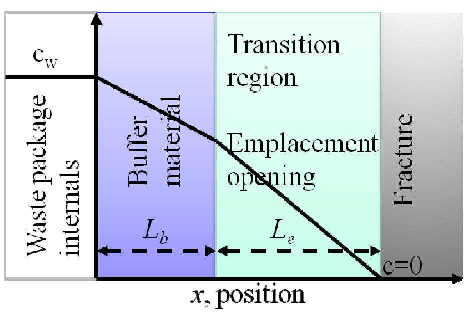

Fig. 2. Concentration versus position at steady state for the one-dimensional, two-leg representation of contaminant transport from the waste package internals to a nearby fracture.

With this simple model, steady diffusive fluxes from the waste package to the flowing fracture reduce to

$$Q = c_w \frac{C_b C_e}{C_b + C_e} \tag{1}$$

$$C_i = \frac{D_i A_i}{L_i} \tag{2}$$

where Q is flux through the transition zone [M/T] (discharge into the fracture), c_w is concentration at the waste package [M/L^3], C_i ($I = b,e$) is conductance [L^3/T], D_i is the diffusion coefficient [L^2/T], A_i is the cross-sectional area for diffusion [L^2], and L_i is the diffusion length [L]. The subscripts b and e represent the buffer and emplacement opening (transition region), respectively. The product of D_i and A_i ($I = b,e$) is uncertain but constrained for both the buffer and emplacement, L_b is typically known from the geometry of the emplacement scheme, and L_e is spatially variable (and uncertain). See Fig. 2 for a geometric representation of L_b and L_e. The objective of the analysis is determining a representative value for L_e, denoted as L_e^o.

The effect of transport distance is isolated by rewriting Eq. (1) with the assumption that C_b, D_e, and A_e are known for a given realization:

$$\frac{Q}{c_w C_b} = \frac{1}{\dfrac{C_b}{C_e} + 1} = \frac{1}{\dfrac{C_b}{C_{f0}}\lambda + 1} \tag{3}$$

where

$$C_{f0} = \frac{D_e A_e}{L_o} \tag{4}$$

$$\lambda = \frac{L_e}{L_o} \tag{5}$$

and L_o is the median fracture spacing [L]. The ratio of C_b to C_{f0} is a useful metric for comparing estimates.

From Eq. (3), the buffer controls transport when $C_b << C_e$ and release is insensitive to the value of the representative parameter (the concentration outside the buffer zone is approximately zero). The representative parameters control release when $C_b >> C_e$, and release is inversely proportional to C_e. Note that transport in the emplacement opening does not limit release for those waste packages sufficiently near a flowing fracture even when the average transport distance is large.

III.A. Representative Transport Length Using Direct Averages (Method 1)

Limitations in selecting a representative parameter are illustrated using arithmetic, harmonic, and geometric averaging to calculate expected fracture separation L_a, L_h, and L_g, respectively, based on the probability distribution for the fracture separation L, $\rho(L)$. L_a, L_h, and L_g are defined by

$$L_a = E[L] = \int_0^\infty \rho(L)\, dL \tag{6}$$

$$L_h = \frac{1}{E[1/L]} = \left(\int_0^\infty \frac{\rho(L)}{L} dL \right)^{-1} \tag{7}$$

$$L_g = \exp\left(E[\ln(L)]\right) = \exp\left(\int_0^\infty \ln(L) \rho(L)\, dL \right) \tag{8}$$

Arithmetic averaging is a common method for developing representative parameters. Harmonic averaging is consistent with the inverse relationship between L_e and the left-hand side of Eq. (3) for $C_b >> C_e$. Geometric averaging provides the most likely value for lognormally distributed variables.

The parameter λ is defined as the ratio of the distance of the waste package to the nearest fracture to the total fracture spacing, or the minimum of *f* and (1−*f*). Because λ is measured with respect to the nearest fracture, its maximum value is 1/2. The waste package can be located anywhere between the fractures; thus, the parameter λ follows a uniform distribution, $0 < \lambda \leq 1/2$, and the expected distance to the nearest fracture is a quarter of the fracture separation (λ = 1/4).

The representative length L_e^o is defined as λL_a, λL_h, or λL_g with λ treated as an adjustable parameter. Fig. 3a illustrates the behavior of the averaging approaches for several sets of lognormally distributed fracture separations, using λ = 1/4 and a range of standard deviations for the fracture separation. Releases are insensitive to fracture separation for $C_b << C_e$, and all approaches have the same relationship in the limit when the fracture spacing approaches zero variance. Reflecting the lognormal distribution, the arithmetic, geometric, and harmonic averaging approaches calculate reduced, unchanged, and greater releases, respectively, as variability in the fracture spacing increases. Fig. 3b, comparing the averages with different λ values, illustrates that changing λ simply shifts the curves horizontally along the *x* axis.

III.B. Equivalent Transport Length by Matching Total Releases (Method 2)

The representative parameter approach by matching total releases considers diffusion-only transport from the waste package to the closest two flowing fractures (see Fig. 1). Each of the two pathways (pathways labeled as Pathway 1 and Pathway 2 in Fig. 1) is modeled as a two-leg system as in Fig. 2. The lengths of Pathways 1 and 2 are denoted as $L_1 = f\,L$ and $L_2 = (1{-}f)\,L$, respectively. The representative length, L_e^o, is defined by the single pathway (as depicted in Fig. 2) that matches the total flux of Pathways 1 and 2. Matching the sum of fluxes through the two pathways to the flux from the equivalent pathway leads to the expression

$$Q = C_b(c_w - c_b) = C_1(c_b - 0) + C_2(c_b - 0) = C_e c_b \qquad (9)$$

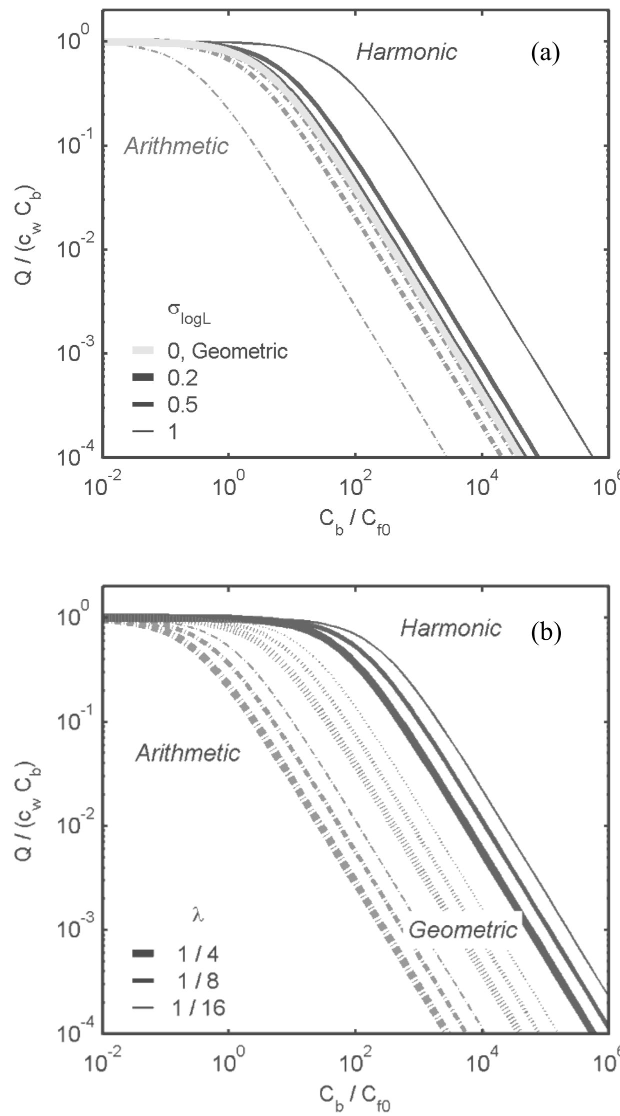

Fig. 3. Normalized releases calculated with averaged fracture separation. (a) Varying standard deviation of log(*L*) (λ = 1/4). (b) Varying λ [standard deviation of log(*L*) = 1].

where c_b is the concentration outside the buffer zone, C_1 and C_2 are the diffusive conductance in pathways 1 and 2 for transition region, and $C_e = C_1 + C_2$ is the total transition region conductance. Assuming that waste package and buffer material dimensions are small compared to the fracture spacing, the total conductance C_e can be approximated as

$$C_e = \frac{D_e A_e}{L}\left(\frac{1}{f} + \frac{1}{1-f}\right) = \frac{D_e A_e}{L\,f(1-f)} \qquad (10)$$

If *L* and *f* are known, Eq. (1) is used to compute the total flux to the flowing fractures. The expected value for the flux, E[Q], accounting for the entire distribution of fracture spacing, L, and waste package placement, f, is computed as

$$\mathrm{E}[Q] = c_w \int_0^\infty \rho(L) \int_0^1 \frac{C_b C_e}{C_b + C_e} \, df \, dL \tag{11}$$

where $\rho(L)$ is the probability density function for the fracture separation. The placement parameter f is assumed to follow a uniform distribution, $0 < f \leq 1$. Expanding C_e and rearranging, expected release is (for a particular realization of all parameters except L)

$$\begin{aligned} \frac{\mathrm{E}[Q]}{c_w C_b} &= \int_0^\infty \rho(L) \int_0^1 \frac{df}{G f(1-f)+1} dL \\ &= \int_0^\infty \rho(L)\, I(G)\, dL \\ &= F \end{aligned} \tag{12}$$

where

$$G = \frac{C_b}{D_e A_e} L \tag{13}$$

$$I(G) = \frac{2}{\sqrt{G(4+G)}} \ln\left(\frac{\sqrt{1+4/G}+1}{\sqrt{1+4/G}-1}\right) \tag{14}$$

The equivalent transport length L_e^o is calculated by combining Eqs. (1), (2), and (12), leading to

$$L_e^o = \frac{D_e A_e}{C_b}\left(\frac{1-F}{F}\right) \tag{15}$$

IV. DISCUSSION

Figs. 4 and 5 illustrate consequences of the representative parameter approach by comparing Method 1 (direct averages) representative-parameter estimates with Method 2 (total release match) representative-parameter estimates for the same fracture set. The Method 2 representative-parameter estimates are qualitatively similar to the harmonic-average estimates from Method 1, in the sense that increased variability leads to larger releases. The Method 2 representative-parameter estimates are qualitatively dissimilar from the arithmetic-average estimates of Method 1, in the sense that the arithmetic-average estimated releases are always smaller than the Method 2 estimated releases and the discrepancy increases with increasing variability.

The Method 1 and Method 2 representative-parameter relationships have differing slopes, even with no variability in fracture spacing (Fig. 4). The Method 2 representative-parameter approach generally exhibits greater calculated release rates, except for harmonic averaging of Method 1 with very large fracture variability (Fig. 5).

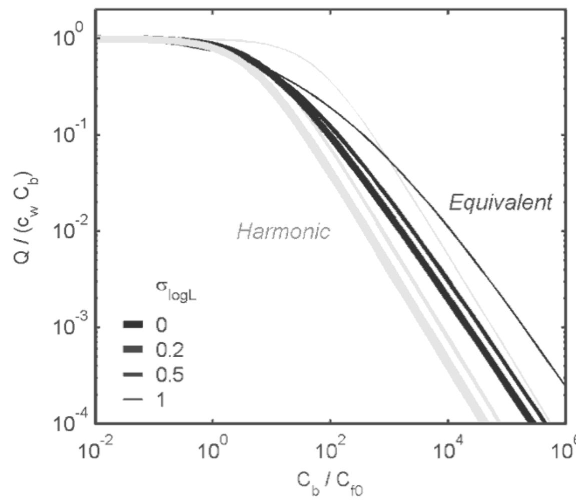

Fig. 4. Normalized releases calculated using Method 2 and harmonic averaging from Method 1 for fracture separation (λ = 1/4).

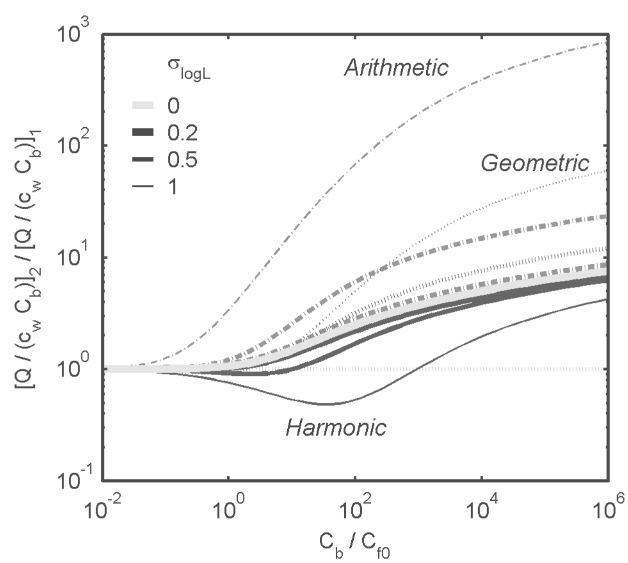

Fig. 5. Ratio of normalized releases calculated using representative parameter approach (Method 2) to arithmetic and harmonic averaging (from Method 1) for fracture separation [λ = 1/4].

Discrepancies between release rates calculated using the various approaches can be removed by adjusting the λ values used for the averaging methods. However, the adjusted λ value depends on the ratio between C_b and C_{f0} (as transport in the transition leg increasingly constrains release, the length of the zone that is effective in contributing to release decreases), implying that the fitted λ value is problem dependent.

These comparisons illustrate that the ultimate use for a parameter may suggest alternative approaches for estimating the parameter. In this case, an arithmetic mean is an unbiased approach for estimating the average fracture separation, but it results in the poorest estimates for releases (the metric of interest). The harmonic mean underestimates the average fracture separation, but is the most appropriate selection because the reciprocal of fracture separation is closely related to the metric of interest. The geometric mean is intermediate to the other two.

This study focused on steady-state or quasi-steady-state considerations. If transient storage effects are taken into account, determination of representative parameters may not be possible without losing detail. For example, total release from an ensemble of waste packages, each simulated accounting for transients, may be well spread in time as the contributions from successively more distal waste packages reach a fracture, while releases from a single representative waste package can only approximate that spread while simultaneously reproducing leading edges. Transient storage effects are also radionuclide dependent in cases where different radionuclides have different sorption patterns or different sorption uncertainties. Thus, a single representative element is constrained to provide limited answers.

This study focused on a single parameter, a length of a transport pathway, L_e. In performing the derivations it was assumed that other parameters, such as concentrations and solubilities, retardation coefficients, and diffusion coefficients, exhibited limited variability. Parameters with wider variability can be considered using nested integrals to compute expected values such as the integrals in Eq. (11) if the variation corresponds to random spatial variability. However, some variability may be correlated to other processes, such as temperature and waste package failure. In that case, it is unlikely that a single representative element can appropriately capture a range of behaviors controlling radionuclide release. A performance assessment model considering those more complex systems may require multiple "representative" elements to capture the increased complexity, with each element capturing a subset of the entire range of behavior.

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REFERENCES

1. C. MARKLEY, E.L. TIPTON, J. WINTERLE, O. PENSADO, and J. GWO, "β-Soar: A flexible tool for analyzing disposal of nuclear waste," *Proceedings of the 2011 International High-Level Radioactive Waste Management Conference (IHLRWM)*, Albuquerque, New Mexico, April 10–14, 2011, *this publication*.
2. J.C. HELTON and C.J. SALLABERRY. "Computational Implementation of Sampling-Based Approaches to the Calculation of Expected Dose in Performance Assessments for the Proposed High-Level Waste Repository at Yucca Mountain, Nevada," *Reliability Engineering and System Safety*, **94** , 699-721 (2009).
3. J.C. HELTON, J.D. JOHNSON, C.J. SALLABERRY, and C.B. STORLIE, "Survey of Sampling-Based Methods for Uncertainty and Sensitivity Analysis," *Reliability Engineering and System Safety*, **91**, 1175–1209 (2006).